10-Undecenoic acid, 3-methylbutyl ester

Other names: iso-Amyl 10-undecenoate
Isopentyl 10-undecenoate
isopentyl undec-10-enoate
Inchi: InChI=1S/C16H30O2/c1-4-5-6-7-8-9-10-11-12-16(17)18-14-13-15(2)3/h4,15H,1,5-14H2,2
InchiKey: DMSGZRWAESVGIP-UHFFFAOYSA-N
Formula: C16H30O2
SMILES: C=CCCCCCCCCC(=O)OCCC(C)C
Mol. weight [g/mol]: 254.41
CAS: 10214-27-4

Physical Properties

Property code	Value	Unit	Source
gf	-64.68	kJ/mol	Joback Method
hf	-498.22	kJ/mol	Joback Method
hfus	35.18	kJ/mol	Joback Method
hvap	59.31	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	4.883		Crippen Method
mcvol	239.440	ml/mol	McGowan Method
pc	1415.44	kPa	Joback Method
rinpol	1717.00		NIST Webbook
rinpol	1717.00		NIST Webbook
ripol	2000.00		NIST Webbook
ripol	2000.00		NIST Webbook
tb	638.01	K	Joback Method
tc	809.72	K	Joback Method
tf	325.48	K	Joback Method
vc	0.930	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.48	J/mol×K	638.01	Joback Method
cpg	671.17	J/mol×K	666.63	Joback Method

cpg	688.07	J/mol×K	695.25	Joback Method
cpg	704.21	J/mol×K	723.86	Joback Method
cpg	719.60	J/mol×K	752.48	Joback Method
cpg	734.26	J/mol×K	781.10	Joback Method
cpg	748.22	J/mol×K	809.72	Joback Method
dvisc	0.0030549	Pa×s	325.48	Joback Method
dvisc	0.0012239	Pa×s	377.57	Joback Method
dvisc	0.0006121	Pa×s	429.66	Joback Method
dvisc	0.0003556	Pa×s	481.75	Joback Method
dvisc	0.0002297	Pa×s	533.83	Joback Method
dvisc	0.0001604	Pa×s	585.92	Joback Method
dvisc	0.0001187	Pa×s	638.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10214274&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume